

Special Issue

Computational Design of Nanostructures and Related Experimental Validation

Message from the Guest Editor

This Special Issue highlights recent advances in computational simulations and experimental characterization in nanomaterials research, covering both independent studies and collaborative innovations. It emphasizes first-principles calculations, molecular dynamics, multiscale modeling, and machine learning applied to designing novel nanomaterials—such as two-dimensional materials, quantum dots, nano-catalysts, ceramics, semiconductors, and crystal structures—with focuses on structure prediction, performance optimization, and mechanism investigation. Additionally, it features breakthrough developments in advanced synthesis, in situ characterization, and performance testing techniques. We especially welcome work integrating computation and experiments that demonstrate the synergy between theoretical predictions and experimental validation. This issue aims to foster communication across computational nanoscience and experimental nanotechnology, promoting the comprehensive development of nanomaterials from fundamental research to practical applications by inviting original research from related fields.

Guest Editor

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Message from the Editor-in-Chief

Nanoscience and nanotechnology are exciting fields of research and development, with wide applications to electronic, optical, and magnetic devices, biology, medicine, energy, and defense. At the heart of these fields are the synthesis, characterization, modeling, and applications of new materials with lower nanometer-scale dimensions, which we call “nanomaterials”. These materials can exhibit unusual mesoscopic properties and include nanoparticles, coatings and thin films, metal–organic frameworks, membranes, nano–alloys, quantum dots, self-assemblies, 2D materials such as graphene, and nanotubes. Our journal, *Nanomaterials*, has the goal of publishing the highest quality papers on all aspects of nanomaterial science to an interdisciplinary scientific audience. All of our articles are published with rigorous refereeing and open access.

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